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Hydrodynamic Scaling and Its Breakdown in Randomly-Networked Liquids of Silica and Silicates

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典型的な無機ガラス形成液体である熔融シリカおよび熔融シリケートでは、その非常に長い粘性緩和時間ゆえに、粘性係数は、分子動力学 (MD) シミュレーションにて算出される有限時間 (有限周波数) での小さな値から、レオロジー実験にて測定される長時間 (ゼロ周波数) での大きな値へと、数桁にわたる増加を示し、かつその増加は、時間 (周波数) の冪乗則で表される。しかし、観測時間が粘性緩和時間に近づくと、冪乗則は破れ、粘性係数は、ゼロ周波数 (無限時間) における有限値へと収束する。高温高圧下にある熔融シリカおよび熔融シリケートの MD シミュレーションから、周波数冪乗則が確認され、さらに、粘性緩和時間が比較的短い場合では、低周波数極限における冪乗則の破れが示唆される。冪乗則の指数 (流体力学的指数) およびその破綻周波数は、粘性係数の振舞いを特徴付け、また、熔融シリカおよび熔融シリケートでは、ランダム・ネットワーク構造により決定される。

1 Introduction

Molten silica (SiO_2) and silicates (e.g. Mg_2SiO_4) are archetypal inorganic glass-forming liquids, and have large shear viscosities. These properties are attributed to the randomly-networked structure consisting of SiO_4 tetrahedra. The slow shear relaxation, typically over tens nanoseconds or longer, is induced by the long-lived current modes which are generated by the strong non-linear coupling of short-lived modes in the random network.

The relation between structure and dynamics is, in general, one of those problems to which molecular dynamics (MD) is a powerful tool. In the cases of the slow shear relaxation in molten silica and silicates, however, the long-lived current modes are hardly tractable by MD simulations. In these cases, MD simulations can provide merely the 'bare' shear viscosity which represents the propagation of the short-lived current modes and has the small magnitude. It is 'renormalized' by the strong mode-coupling to the 'dressed' shear viscosity which represents the propagation of the long-lived current modes and has the large magnitude.

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2 Hydrodynamic Scaling

2.1 Frequency-Scale Invariance and Hydrodynamic Exponents

In his recent studies, Takéuchi suggests the theory of hydrodynamic scaling to implement the renormalization of the bare shear viscosity at finite frequency (or, finite time) to the dressed shear viscosity at zero frequency (or, infinite time) [1]. The bare shear viscosity, $K_T(k, \omega)$ at finite wavenumber k and finite frequency ω , is coarse-grained in ω -domain by integrating its convolution to the Lorentzian window, $(1/\pi)\Gamma/(\omega^2 + \Gamma^2)$, of the finite half-width Γ . Its approach to the limit $\omega \rightarrow 0$ is then inferred from the hierarchy with decreasing Γ , and is expressed by a power law, Γ^{-w_T} . A 'hydrodynamic' exponent w_T is thus defined and characterizes the behaviors of the dressed shear viscosity. The power law is attributed to the scale invariance (or, self-similarity) in time or frequency [2], by interpreting the long shear relaxation time as diverging to infinity relative to the cut-off time $1/\Gamma$.

2.2 Break-Down of Frequency-Scale Invariance

The frequency-scale invariance, and therefore the power law, break down in the limit $\Gamma \rightarrow 0$, since the shear relaxation time is no longer infinite time relative to $1/\Gamma$. The convergence to the finite magnitude of the dressed shear viscosity is accordingly realized.

Applying the theory of hydrodynamic scaling to $K_T(k, \omega)$ computed from MD simulations on some cases of molten silica and silicates at high temperatures and high pressures, the power law is confirmed. w_T differs by composition, and changes with pressure differently by composition. These differences indicate those in the dressed shear viscosity and in its pressure-dependence. Furthermore, the break-down of the power law is indicated in some cases of less-networked liquids having the relatively short shear relaxation time, and indicates the convergence to the dressed shear viscosity. These behaviors are determined by the randomly-networked structure, the degree of connectivity in which differs by composition and changes with pressure differently by composition.

References

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- [2] P.C. Hohenberg and B.I. Halperin, *Rev. Mod. Phys.*, **49**, 435-479 (1977)